Coastal Ocean Data Analysis Product in North America (CODAP-NA)

This data package contains two folders:

- "Data_CODAP" has four subfolders: CSV, MATLAB, NetCDF, XLSX, each containing the same CODAP-NA data product file in their respective format.
- "Table_QC_changes" contains an Excel spreadsheet documenting all of the QC related changes during the CODAP-NA quality control process.

For more details about this data product, please refer to:

Jiang, L.-Q., Feely, R. A., Wanninkhof, R., Greeley, D., Barbero, L., Alin, S., Carter, B. R., Pierrot, D., Featherstone, C., Hooper, J., Melrose, C., Monacci, N., Sharp, J., Shellito, S., Xu, Y.-Y., Kozyr, A., Byrne, R. H., Cai, W.-J., Cross, J., Johnson, G. C., Hales, B., Langdon, C., Mathis, J., Salisbury, J., and Townsend, D. W.: Coastal Ocean Data Analysis Product in North America (CODAP-NA) – An internally consistent data product for discrete inorganic carbon, oxygen, and nutrients on the U.S. North American ocean margins, Earth Syst. Sci. Data Discuss., https://doi.org/10.5194/essd-2020-402, in review, 2021.

Table 1. Parameters that are included in the data product. CTD is short for conductivity, temperature, and depth, and refers to a package of electronic instruments that measure these properties.

Abbreviation	Variable name		Measured/ calculated
Accession	The data package identification number used by NOAA's Naitional Centers for Environmental Information. This ID can be used to retrieve the original cruise data files.		-
EXPOCODE	Expedition code of a research cruise		-
Cruise_flag	Flags indicating the overall quality of a cruise data file (refer to Table 2 for more details)	-	-
Cruise_ID	The identification of a research cruise	-	-
Observation_type	Whether a sample is collected from Niskin bottles or an onboard flow-through system	-	-
Profile_number	A series of sequential number profile identing a profile	-	-
Station_ID	Identification of a sampling station	-	-
Cast_number	Cast number at a sampling station	-	-
Niskin_ID	Niskin identification number	-	-
Sample_ID	Sample_ID is a combination of Station_ID, Cast_number, and Niskin_ID. Sometimes it can also be a serious of non-repeating numbers to identify each row from a cruise data file.		-
Depth_bottom	Depth at bottom of a sampling station	m	measured
Max_sample_depth	The maximum sampling depth	m	measured
CTDPRES	Water pressure recorded from sensors on a CTD rosette. For surface samples collected from an onboard flow-through system, its pressure is equal to the depth of the water inlet. When such info is not available, it is assumed to be 5 dbar.	dbar	measured
Depth	The depth at which a sample is collected		measured
CTDTEMP_ITS90	Temperature on the International Temperature Scale of 1990 (ITS-90) from sensors on a CTD rosette. For surface samples collected from an onboard flow-through system, temperature has also been merged into the CTDTEMP_ITS90 variable.		measured
CTDSAL_PSS78	Salinity on the Practical Salinity Scale 1978 (PSS-78) from sensors on a CTD rosette. For surface samples collected from an onboard flow-through system, salinity from the thermosalinograph (TSG) has been merged into the CTDSAL_PSS78 variable.		measured
Salinity_PSS78	Discrete salinity on the PSS-78 scale	-	measured
recommended_Salinity_PSS78	Discrete salinity with some missing values filled in using CTDSAL	-	measured
CTDOXY	Dissolved oxygen from sensors on a CTD rosette	μmol kg ⁻¹	measured
Oxygen	Discrete dissolved oxygen from Winkler titration	μmol kg ⁻¹	measured
recommended_Oxygen	Discrete dissolved oxygen from Winkler titration with some missing values filled in using		measured
AOU	Apparent oxygen utilization	μmol kg ⁻¹	calculated
DIC	Dissolved inorganic carbon	μmol kg ⁻¹	measured
TALK	Total alkalinity	μmol kg ⁻¹	measured
pH_TS_measured	pH on total hydrogen scale (TS) at measurement temperature and ambient pressure	-	measured
TEMP_pH	Temperature of pH measurement	°C	measured
pH TS insitu measured	pH on total hydrogen scale (TS) adjusted to in-situ conditions	-	measured
pH_TS_insitu_calculated	pH on total hydrogen scale (TS) at in-situ conditions calculated from DIC, TA and others using CO2SYS	-	calculated
Carbonate_measured			measured
TEMP_Carbonate	Temperature of carbonate ion measurement	μmol kg ⁻¹ °C	measured
Carbonate insitu measured	Carbonate ion at in-situ conditions adjusted to in-situ conditions	μmol kg ⁻¹	measured
Carbonate insitu calculated	Carbonate ion at in-situ conditions calculated from DIC, TA and others using CO2SYS	μmol kg ⁻¹	calculated
fCO ₂ measured	Fugacity of carbon dioxide at measurement temperature and ambient pressure	μatm	measured
J = = <u>z_</u>	g , sampenanc and amount pressure	F	

	-		
TEMP_fCO ₂	Temperature of fCO ₂ measurement		measured
fCO ₂ _insitu_measured	Discrete fugacity of carbon dioxide adjusted to in-situ conditions		measured
fCO ₂ _insitu_calculated	Fugacity of carbon dioxide at in-situ conditions calculated from DIC, TA and others using CO2SYS	μatm	calculated
Aragonite	Aragonite saturation state at in-situ conditions calculated from DIC, TA and others using CO2SYS	-	calculated
Calcite	Calcite Calcite saturation state at in-situ conditions calculated from DIC, TA and others using CO2SYS - calculate		calculated
Revelle_Factor	Revelle Factor calculated from DIC, TA and others using CO2SYS	-	calculated
Silicate	Silicate	μmol kg ⁻¹	measured
Phosphate	Phosphate	μmol kg ⁻¹	measured
Nitrate	Nitrate	μmol kg ⁻¹	measured
Nitrite	Nitrite	μmol kg ⁻¹	measured
Nitrate_and_Nitrite	Nitrate and Nitrite combined	μmol kg ⁻¹	measured
recommended_Nitrate_and_Nitrite	Nitrate_and_Nitrite, along with Nitrate when Nitrate_and_Nitrite data are not available	μmol kg ⁻¹	measured
Ammonium	Ammonium	μmol kg ⁻¹	measured

Table 2. Cruise flags used for this product.

Flag value	Meaning		
A	These are dedicated OA cruises that are executed following Best Practices for global ocean work as outlined in Hood et al. (2011) and other documents as can be found on GO-SHIP site. Colloquially these are referred to as GO-SHIP quality. Traceable standards and certified reference materials are used and deep stations (≈> 2500 m) are executed to be able to use near constant deep-water concentrations as anchor points. A third inorganic carbon system parameter, such as pH or carbonate ion concentration are often measured, allowing consistency checks.		
В	These are dedicated OA cruises that have onboard inorganic carbon measurements performed according to Best Practices (Dickson et al. 2007), and many other parameters to highest accuracy through use of standards and certified reference materials. However, the cruises do not necessarily have all other parameters analyzed to highest standards, such as freezing nutrients for shoreside analyses; not taking oxygen and nutrients samples on most Niskins; not normalizing CTD/O2 trace to Winkler oxygens, insufficient metadata etc. There often are insufficient deep stations to compare data with open ocean data.		
С	These are opportunistic cruises where OA parameters are measured in the water column. They include standard hydrographic, carbon, and OA parameters; T, S, O2, nutrients, TALK,DIC, pH. Many parameters, including carbon and OA parameters are measured shoreside; CTD oxygen are not adjusted to Winkler oxygen. Generally, no dedicated OA personnel are onboard.		
D	Underway samples only. These cruises have no CTD casts and only have samples taken from the seawater supply line with ofter a limited amount of other hydrographic parameters. T and S are obtained from thermosalinographs with limited or no salinity check samples.		

Table 3. World Ocean Circulation Experiment (WOCE) World Hydrographic Program (WHP) (Joyce and Corry, 1994; Swift and Diggs, 2008) QC flags used for this product.

Flag value	Meaning
2	Acceptable
3	Questionable
6	Average of duplicates
9	Missing value

Methods

When discrete salinity and CTDSAL were merged, data were preferentially chosen from the discrete measurements, provided the QC flag is equal to 2 or 6. The same principles were applied to the oxygen data combination. After merging, all missing values are replaced with "-999". The merged variables are called "recommended_Salinity_PSS78" and "recommended_Oxygen", respectively (Table 2).

Apparent oxygen utilization (AOU) was calculated based on absolute salinity, conservative temperature, latitude, longitude, pressure, and recommended_Oxygen variable using the function "gsw_O2sol" as described in the International Thermodynamic Equation of Seawater 2010 (TEOS-10) (IOC et al., 2010). Oxygen solubility is the "combined equation: from Garcia and Gordon (1992).

fCO2_insitu_calculated, Carbonate_insitu_calculated, pH_TS_insitu_calculated, aragonite saturation state, calcite saturation state, and Revelle Factor were calculated from *in-situ* temperature, salinity, DIC, TA, silicate, and phosphate using the MATLAB version (Sharp et al., 2020) of the CO2SYS program (Lewis and Wallace, 1998), with the dissociation constants for carbonic acid of Lueker et al., (2000), bisulfate (HSO₄⁻) of Dickson (1990), hydrofluoric acid (HF) of Perez and Fraga (1987), and with the total borate equations of Lee et al., (2010).

References

- Dickson, A. G.: Standard potential of the reaction: AgCl(s) + 1/2 H2(g) = Ag(s) + HCl(aq), and the standard acidity constant of the ion HSO_4^- in synthetic seawater from 273.15 to 318.15K, J. Chem. Thermodyn., 22, 113–127, doi: 10.1016/0021-9614(90)90074-z, 1990.
- IOC, SCOR, & IAPSO: The international thermodynamic equation of seawater 2010: Calculation and use of thermodynamic properties, Intergovernmental Oceanographic Commission, UNESCO (English), pp. 196pp, 2010.
- Lewis, E., and Wallace, D.W.R. (1998). Program Developed for CO₂ System Calculations, ORNL/CDIAC-105 (Carbon Dioxide Information Analysis Center, Oak Ridge National Laboratory, U. S. Department of Energy, Oak Ridge, Tennessee).
- Lueker, T. J., Dickson, A. G. and Keeling, C. D.: Ocean pCO₂ calculated from dissolved inorganic carbon, alkalinity, and equations for K1 and K2: validation based on laboratory measurements of CO₂ in gas and seawater at equilibrium, Mar. Chem., 70, 105–119, 2000.
- Perez, F. F. and Fraga, F.: Association constant of fluoride and hydrogen ions in seawater, Mar. Chem., 21, 161-168, doi: 10.1016/0304-4203(87)90036-3, 1987.
- van Heuven S., Pierrot, D., Lewis, E., and Wallace, D. W. R.: Matlab Program Developed for CO₂ System Calculations, Carbon Dioxide Information Analysis Center, Oak Ridge National Laboratory, US Department of Energy, Oak Ridge, Tennessee, 2009.
- Lee, K., Kim, T.-W., Byrne, R. H., Millero, F. J. Feely, R. A., and Liu, Y.-M.: The universal ratio of boron to chlorinity for the North Pacific and North Atlantic oceans, Geochimica et Cosmochimica Acta, 74, 1801-1811, https://doi.org/10.1016/j.gca.2009.12.027, 2010.
- Sharp, J.D., Pierrot, D., Humphreys, M.P., (2020). CO2-System-Extd, v3.0.1, MATLAB (MathWorks), http://doi.org/10.5281/zenodo.3952803, 2020.